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PATENT



IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

In re application of:

Dath et al

Serial No.:

09/205,056

Filed:

December 3, 1998

Group Art Unit:

1764

Examiner:

B. Yildirim

For:

PRODUCTION OF PROPYLENE

Via First Class Mail

Assistant Commissioner for  
Patents  
Washington, DC 20231

Sir:

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Clare Jackson August 13, 2001  
Clare Jackson Date of Deposit

APPEAL BRIEF

This is an appeal from the decision of the Primary Examiner finally rejecting claims 1-9, 12, and 13. This Brief is submitted in triplicate with the statutory fee of \$310.00.

Real Party in Interest

The real party in interest is Fina Research, S.A., a Belgium corporation, as recorded by the assignment dated March 2, 1999, and recorded in the Patent and Trademark Office on March 22, 1999, at Reel 9843 / Frame 0252.

### **Related Appeals and Interferences**

There are presently no appeals or interferences which are directly related to this appeal. However, commonly-assigned Application Serial No. 09/206,218, having the same inventive entity as this application and directed to a process for increasing the stability of an MFI-type silicate catalyst and a process for the catalytic cracking of olefins, is the subject of an appeal filed March 29, 2001. Also, commonly-assigned Application Serial No. 09/206,210, directed to a process for the cracking of an olefinic feedstock over an MFI-type silicate is the subject of an appeal filed May 2, 2001.

### **Status of Claims**

The claims pending in this application are claims 1-9, 12, and 13. Claims 1-9, 12, and 13 are appealed and are reproduced in Exhibit A. No claim is allowed.

### **Status of Amendments**

An Amendment Under 37 CFR 1.116 was filed on June 13, 2001, and according to the Advisory Action of June 28, 2001, this Amendment will be entered upon the filing of this Appeal Brief.

### **Summary of the Invention**

The invention called for in the claims on appeal involves a conversion process for the production of propylene by the cracking of an olefinic feedstock containing at least one olefin having 4 or more carbon atoms. The olefin is contacted with an MFI-type catalyst, specifically silicalite or ZSM-5, which has a silicon/aluminum atomic ratio of from 180 to 1000 to produce a

product having propylene which is in the amount of from 30-50% of the olefinic content of the feedstock. The catalyst used in the process has been pretreated by heating the catalyst in steam followed by a de-alumination treatment in which the catalyst is contacted with a complexing agent for aluminum. This treatment removes amorphous alumina produced during the steaming step from the catalyst framework as described in appellants' specification in the paragraph bridging pages 13 and 14. This enables the cracking process to proceed within the pores of the MFI-type catalyst to provide a high propylene yield with an enhanced stability of the MFI catalyst over time.

The MFI catalyst employed in appellants' invention, which has been dealuminated by removal of aluminum from the pores of the framework, is of a particular crystalline structure type as established by the Structure Commission of the International Zeolite Association, as referred to on page 1 of appellants' specification. As stated there, ZSM-5 and silicalite are MFI-type crystalline silicates. Attached hereto as Exhibit B is a copy of pages 1-12, and 89-93 from the *Atlas of Zeolite Structure Types* by Meier et al, published by the Structure Commission of the International Zeolite Association in 1978. As indicated on page 93, ZSM-5 and silicalite (referred to in Footnote 1 by reference to Flanigen et al (1978)) are MFI-structure types.

The effect of the steaming and dealumination procedure specified in appellants' claims is to remove aluminum from throughout the crystalline framework structure. This is described in the paragraph bridging pages 13 and 14 of the specification by reference to a typical commercially-available silicalite initially having a silicon/aluminum atomic ratio of about 120 (corresponding to a silica/alumina ratio of 240). The steaming step functions to reduce the tetrahedral aluminum in the crystalline framework to the form of amorphous alumina. The subsequent treatment with the complexing agent functions to remove the amorphous alumina

from the pores of the silicate framework so that dealumination occurs internally throughout the whole pore surfaces of the catalyst to increase the framework silicon/aluminum atomic ratio to a value of at least 180 (corresponding to a silica/alumina ratio of 360).

### **Prior Art**

The prior art reference relied upon in rejecting the claims under 35 U.S.C. § 103 is EP 019060 to Colombo.

### **Issues**

The issue in this appeal is whether claims 1-9, 12, and 13 are patentable over EP 109060 to Colombo.

### **Grouping of Claims**

In the arguments presented in this Brief, all of the claims do not stand and fall together. In addition to the arguments with respect to independent claim 1, which are of course applicable to all of the claims, additional arguments are presented with respect to each of claims 2, 3, and 4. Further, additional arguments are presented with respect to each of claims 5, 6, 7, and 9.

### **Appellants' Arguments**

Appellants' independent claim 1 is directed to a cracking process for the production of propylene from an olefinic feedstock which distinguishes over EP '060 to Colombo in several important respects. First of all, the appellants' process requires the use of an MFI-type catalyst having a silicon/aluminum ratio of from 180 to 1000. EP '060 discloses a wide variety of

catalysts, some of which, ZSM-5 and silicalite, would appear to be MFI catalysts; others of which are not. For this broad group of catalysts, EP '060 simply specifies a silicon/aluminum ratio greater than 175, thus including catalysts in which no aluminum is present. To the extent an MFI-type catalyst, silicalite, is disclosed, the reference specifically calls for a silicon/aluminum ratio of infinity, that is, with no aluminum present in the silicate. EP '060 further fails to disclose the use of a catalyst as claimed to produce a propylene yield on an olefin basis of 30-50% of the olefinic content of the feedstock. Finally, EP '060 fails completely to disclose the all-important step of employing a catalyst which has been pretreated by heating the catalyst in steam to dealuminate the catalyst by forming amorphous alumina followed by a treatment of the catalyst with a complexing agent for aluminum in order to remove amorphous alumina from the pores of the catalyst to increase the silicon/aluminum atomic ratio of the catalyst to a value of from 180 to 1000. The Examiner in the Advisory Action of June 28, 2001, seeks to dismiss this claimed subject matter in evaluating patentability of the claims on the grounds that this is a preferred embodiment. With respect to this subject matter, as well as the other subject matter in appellants' claimed procedure which is not disclosed in EP '060, appellants would respectfully submit the issue is one of novelty and obviousness to one of ordinary skill in the art in view of the reference. The fact that this may be denominated in appellants' specification as a preferred embodiment (which has been claimed in this application since its filing) does not, appellants would respectfully submit, relieve the Examiner of the obligation to establish obviousness of the claimed subject matter. As I discussed below, the subject matter claimed is clearly not obvious in view of the EP '060 reference.

The Examiner apparently concedes that EP '060 does not disclose the use of a steamed and dealuminated MFI-type catalyst in the cracking of an olefin stream to produce propylene in

the effluent in an amount within the 30-50% range as specified in the claims. Contrary to the comments made in the Advisory Action of June 28, 2001, the use of a catalyst which has been pretreated by steam and dealumination with a complexing agent must be considered as it is specifically recited in independent claim 1. To the extent that the Examiner would argue that this claim limitation can be given weight only if it produces an unexpected result, appellants would respectfully disagree. As noted previously, the issue is one of novelty and unobviousness. It is clear that the use of the catalyst as specified in claim 1 is novel in view of the '060 patent, and further, it is unobvious. In fact, there is nothing in the '060 patent which would even remotely suggest the use of an MFI-type catalyst which has been pretreated as called for in claim 1.. There clearly is no issue of a *prima facie* case of obviousness which would bring into play the question of unexpected results resulting from use of a catalyst which has been subject to steaming and dealumination as specified in the claim.

Further, it is respectfully submitted that the data in appellants' specification clearly shows the presence of unexpected results stemming from the use of a catalyst as required in claim 1. In this regard, attention is respectfully invited to a comparison of Example 1 (with results reported in Table 1, page 25, and Fig. 1) and Example 10 (with results reported in Fig. 2). In Example 1, the silicalite catalyst having a silicon/aluminum ratio of 220 was subject to a steaming and dealumination extraction procedure employing EDTA to increase the silicon/aluminum ratio from 220 to 280. As indicated, the catalyst exhibited good stability to propylene yield over a test period of 325 hours. In contrast, in Example 10 the result was a much more dramatic decrease in activity over a slightly shorter period of time employing a silicalite catalyst which was the same as the starting catalyst (silicon/aluminum ratio of 220) subject to the steaming and dealumination step and used in Example 1. Similar good results resulting from the use of silicalite catalyst

subject to steaming and dealumination are shown in other examples set forth in appellants' specification. For example, Example 8, with the results reported in Table 12a shows the results of cracking of a butene-containing feedstock employing a steamed and dealuminated silicalite following the procedure of Example 4 and having a silicon/aluminum atomic ratio of 180. As indicated in Table 12a, at 164 hours the propylene yield showed absolutely no degradation from measurements taken at 20 hours. This result may be contrasted with the results shown in Tables 12b and 12c, respectively, for the starting silicalite catalyst and the starting silicalite catalyst steamed but not subject to extraction. As set forth in Tables 12b and 12c, the propylene yield fell off rapidly at 169 hours in Table 12b and showed a substantial decline also in Table 12c.

The issue of pretreating aside, as noted above EP '060 does not disclose contacting an olefinic feedstock with an MFI-type catalyst having a silicon/aluminum atomic ratio of from 180 to 1000. EP '060 discloses a number of catalysts, some of which presumably are MFI-type catalysts and others which clearly are not. For example, EP '060 discloses the use of ZSM-5, silicalite (of a silica/alumina ratio well above the 180-1000 range), and ZSM-11. For the purpose of this appeal, it is presumed that the Silicalite I and the ZSM-5 zeolite disclosed in EP '060 are MFI crystalline silicates. Another catalyst disclosed in EP '060, ZSM-11, clearly is not an MFI-type silicate. In this regard, attention is respectfully invited to the aforementioned "Atlas of Zeolite Structure Types," attached as Exhibit B, and particularly the structure-type index appearing on pages 89-93 thereof. As shown there, ZSM-11 is of structure-type MEL. Various other catalysts disclosed in EP '060 may or may not be MFI-type zeolites; it is simply impossible to tell. The Silicalite 1 actually disclosed in EP '060 clearly does not have a silicon/aluminum atomic ratio of from 180 to 1000 as called for in appellants' claims. In fact, to the extent that the silicon/aluminum atomic ratio is addressed in EP '060, the reference simply requires a ratio of at

least 175 and actually discloses an MFI-type catalyst (silicalite) in which no aluminum is present. In fact, every example in EP '060 addressing silicalite specifies a silicon/aluminum ratio of infinity, *i.e.* no aluminum is present. Thus, a fair reading of the disclosure in EP '060 is that the silicon/aluminum atomic ratio is of no significance, and it makes no difference whether or not aluminum is even present in the catalyst.

In addition to the requirement in appellants' claim 1 of an MFI-type catalyst having a silicon/aluminum atomic ratio of 180 to 1000 produced by steaming and complexing agent pretreatment, EP '060 further fails to disclose a process carried out to provide a propylene yield of from 30-50% based upon the olefinic content of the feedstock. To the extent the Final Rejection would argue that this result of a propylene yield within the 30-50% range would "flow naturally" from the operation of the reference, appellants would respectfully disagree. The data presented in EP '060 for the various examples given there is somewhat sparse and is presented without elaboration. Thus, it is difficult to determine precisely what the propylene yield, in terms of the olefinic content of the feedstock, would be. However, one example, Example 36, does present in Fig. 1 the results of experimental work carried out employing Silicalite I as the catalyst and a feedstock of a 50/50 mixture of cis-butene-2 and trans-butene-2 over a period of 120 hours. While the silicon/aluminum atomic ratio of the Silicalite I of Example 36 is not given, it is noted that in the other examples employing silicalite, the silicon/aluminum ratio was necessarily greater than 1000. The results of Example 36 are presented in Fig. 1 of EP '060. As indicated there, the propylene content of the converted feed, as indicated by the selectivity to propylene, is less than 30% over the life of the run. The conversion of the olefinic feed ranges from about 68% to a maximum of about 80% initially and generally is about 75% until it starts to fall off after about 80 hours on stream. Throughout the test run, the propylene content (the



product of conversion and selectivity) is clearly less than 25% based upon the olefinic content of the feedstock, which, of course, is 100%. Thus, based upon the data presented in Example 36, the conclusion clearly is that the propylene content is below the 30-50% range called for in appellants' claims.

Aside from the data presented in Example 36 of EP '060, to the extent that the Examiner's rejection is based upon an argument of inherency, appellants would respectfully note that the law is well settled that for an alleged inherent feature to result from a prior art teaching, it is necessary that this inherent feature necessarily flow from the teachings of the prior art. Thus, an alleged inherent feature must be a necessary result and not merely a possible result. This principle is stated in MPEP Section 2112:

The fact that a certain result or characteristic may occur or be present in the prior art is not sufficient to establish the inherency of that result or characteristic. (Emphasis original)

Section 2112 reflects the general rule that for inherency to reside, it must be shown that the alleged inherency is necessarily present and not a mere possibility. Thus, as stated by the Board in *Ex parte Keith*, 154 USPQ 321 (Bd. of App. 1966), in reversing the Examiner's rejection based upon inherency:

There are other possible courses the reaction could follow . . . Asserted inherency must be a necessary result and not merely a possible result.

As indicated in Section 2112, this principle was more recently followed by the Board in *Ex parte Levy*, 17 USPQ2d 1461 (Bd. of App. and Interf. 1990), where the Board reversed an inherency rejection, stating as follows:

In relying upon the theory of inherency, the examiner must provide a basis in fact and/or technical reasoning to reasonably support the determination that the alleged inherent characteristic necessarily flows from the teachings of the prior art (citing cases). (emphasis original).

Here, the issue presented by the rejection based upon EP '060 is not only the requirement for a propylene yield of 30-50% but also the requirement that the catalyst employed in the cracking process be one which is pretreated by steaming and dealumination with a complexing agent for aluminum in which the silicon/aluminum atomic ratio of the catalyst is from 180 to 1000. This combination of features is not disclosed or suggested in the EP '060 reference, and it is clearly not inherent therein.

In addition to the foregoing arguments, which are applicable to all of the claims, appellants would respectfully submit that each of claims 2, 3, and 4 are directed to use of feedstocks in appellants' invention which are not disclosed or suggested in EP '060. It is noted that EP '060 discloses in the paragraph bridging pages 3 and 4 the treatment of the output from a catalytic cracking unit for use as the feedstock in the conversion process. Apparently, in this case the feedstock would be subjected to an oligomerization procedure to produce a feed stream of C<sub>5</sub>-C<sub>8</sub> olefins and C<sub>4</sub>+ paraffins. It is respectfully submitted that this disclosure would not suggest or render obvious the use of the specific feedstocks specified in dependent claims 2, 3, and 4.

Dependent claim 5 calls for at least 95% of the C<sub>3</sub> compounds in the effluent to be propylene. Again referring to Example 36 as discussed above, it is noted that Fig. 1 discloses data over the course of the run for selectivity to liquids (C<sub>5</sub> and greater) and selectivity to saturated gases which presumably would include gases of less than C<sub>5</sub>, specifically including propane. The selectivity to propylene is over most of the run about 7 to 8 times the selectivity to

saturated gases, and thus it is clear that saturated  $C_3$  content of the effluent could be well in excess of 5%, leaving the propylene content at less than 95%.

Appellants' dependent claim 6 specifies that the feedstock contacts the catalyst at an inlet temperature of 500-600°C, and claim 7 depends from claim 6 and specifies an inlet temperature of 540-580°C. Dependent claim 9 specifies that the feedstock contacts the catalyst or is passed over the catalyst at a liquid hourly space velocity (LHSV) of from 10-30  $h^{-1}$ . EP '060 does not disclose or suggest this particular combination of parameters and instead discloses, in addition to the very broad range of the silicon/aluminum ratio, broad ranges of olefin partial pressure, space velocity, and temperature. Thus, EP '060 specifies a temperature of 400-600°C and a space velocity of 5-200  $hrs.^{-1}$ . Thus, while EP '060 discloses broad ranges of these parameters within which more specific values could be selected, the particular combination of the silicon/aluminum atomic ratio with the inlet temperature, as specified in claims 6 and 7, and space velocity, as set forth in claim 9, can be arrived at only by selecting these values from the broad ranges in EP '060 based upon appellants' disclosure. In fact, with respect to space velocity as set forth in dependent claim 9, the only qualification of space velocity as described in EP '060 appears to be that the space velocity should be less than 50  $hrs.^{-1}$  if the pressure is atmospheric and greater than 50  $hrs.^{-1}$  at a pressure of from 1.5 to 7.5 atmospheres. As a practical matter, EP '060 suggests as a whole that the space velocity should be outside the 10-30  $hrs.^{-1}$  range specified in appellants' dependent claim 9. An exception to this is found in the aforementioned Example 36 of EP '060, but here a silicon/ aluminum atomic ratio of infinity (silicalite totally free of aluminum), rather than within the range of 180 to 1000, and a propylene yield well below the 30-50% value as called for in appellants' claims, are involved. There is simply nothing in EP '060 which

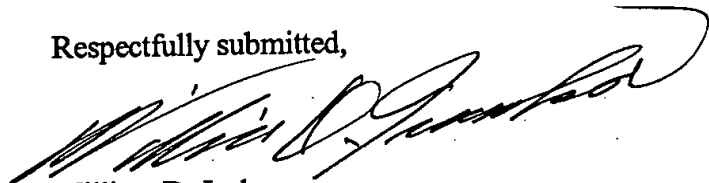
discloses or renders obvious the combination of silicon/aluminum ratio, propylene yield, and space velocity as called for in the claims as indicated above.

### Conclusion

For the reasons set forth above, Appellants respectfully submit that all of the claims herein are patentable over the prior art. Accordingly, it is respectfully requested that the Final Rejection of the claims be reversed.

Enclosed is a check in the amount of \$310.00 to cover the fee for the filing of this Appeal Brief. The Commissioner is hereby authorized to charge any additional fees that may be due in connection with this Appeal Brief to Deposit Account No. 12-1781.

Respectfully submitted,



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Date: August 13, 2001

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**CLAIMS ON APPEAL**

1. A process for the production of propylene from an olefinic feedstock containing at least one olefin of C<sub>4</sub>, or greater, the process comprising contacting the olefinic feedstock with a catalyst of the MFI-type having a silicon/aluminum atomic ratio of from 180 to 1000 to produce an effluent containing propylene, the propylene yield on an olefin basis being from 30 to 50% based on the olefinic content of the feedstock, wherein the catalyst has been pretreated by heating the catalyst in steam and de-aluminating the catalyst by treating the catalyst with a complexing agent for aluminum, the pretreatment increasing the silicon/aluminum atomic ratio of the catalyst to a value from 180 to 1000.

2. A process according to claim 1, wherein the feedstock comprises a light cracked naptha.

3. A process according to claim 1, wherein the feedstock is selected from the group consisting of a C<sub>4</sub> cut from a fluidised-bed catalytic cracking unit in a refinery, a C<sub>4</sub> cut from a unit in a refinery for producing methyl tert-butyl ether, and a C<sub>4</sub> cut from a steam-cracking unit.

4. A process according to claim 1, wherein the feedstock is selected from the group consisting of a C<sub>5</sub> cut from a steam cracker and light cracked naptha.

5. A process according to claim 1, wherein at least 95 wt.% of any C<sub>3</sub> compounds in the effluent are present as propylene.

6. A process according to claim 1, wherein the feedstock contacts the catalyst at an inlet temperature of from 500 to 600°C.

7. A process according to claim 6, wherein the inlet temperature is from 540 to 580°C.

8. A process according to claim 1, wherein the feedstock contacts the catalyst at an olefin partial pressure of from 0.1 to 2 bar.

9. A process according to claim 1, wherein the feedstock is passed over the catalyst at an LHSV of from 10 to 30h<sup>-1</sup>.

12. A process according to claim 1, wherein the catalyst of the MFI-type is of the silicalite type.

13. A process according to claim 1, wherein the catalyst of the MFI-type is of the ZSM-5 type.

***Exhibit B***

Structure Commission  
of the International Zeolite Association

ATLAS OF ZEOLITE STRUCTURE TYPES

by

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Structure type data sheets with stereopairs (in alphabetical order according to the structure type codes)

ABW	AFG	ANA	BIK
BRE	CAN	CHA	DAC
EAB	EDI	EPI	ERI
FAU	FER	GIS	GME
HEU	KFI	LAU	LEV
LIO	LOS	LTA	LTL
MAZ	MEL	MER	MFI
MOR	NAT	OFF	PAU
PHI	RHO	SOD	STI
THO	YUG		

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## PREFACE

The steadily growing number of known zeolite structures and numerous requests which have been received for a previous survey of zeolite framework types has led to the present "Atlas of Zeolite Structure Types". The primary aim of the present compilation is to define and to supply a condensed characterization of the 38 currently established zeolite structure types. Apart from the stereopairs illustrating the framework structures the Atlas contains summaries of structural data as well as a Structure Type Index that includes all natural and synthetic materials which have been shown to be an isotype of a known zeolite structure type.

The present Atlas contains only reasonably well-established structures which have been at least partially refined. A number of zeolite structures included are by necessity based on powder data. A total of 38 structure types could, after critical assessment of the respective structure analysis, be included in this Atlas (compared to 27 in the previous survey by Meier and Olson, 1971).

Zeolites do not comprise an easily definable family of crystalline aluminosilicates. The inclusion or exclusion of borderline cases was decided on the basis of criteria used at recent International Conferences on zeolites.

We wish to acknowledge the use of the stereographic computer plotting program ORTEP, written by Dr. Carroll K. Johnson (Oak Ridge National Laboratory). A listing of the ORTEP input used to generate the stereopairs in this Atlas has been deposited as document number NAPS-03331. (Order from ASIS/NAPS, Microfilm Publications, P. O. Box 3513, Grand Central Station, New York, N. Y. 10017). Information obtained by private communication in addition to the published data has in several instances been used in the preparation of the Atlas. Such use is indicated in the References and we gratefully acknowledge this help. We also wish to thank our colleagues of the IZA Structure Commission for critically

reading the manuscript and many helpful comments. Furthermore, we are grateful for the support by Mobil Research and Development Corporation and one of us (D. H. O.) is also indebted to this company for permission to participate in this project. The work of the other author (W. M. M.) has been part of a research program supported by the Swiss National Science Foundation.

## Explanatory Notes

Probably the simplest way of illustrating zeolite structures is by means of skeletal models or diagrams showing the 4-connected nets formed by the tetrahedral atoms in the various aluminosilicate frameworks. The known zeolite framework types are presented in this Atlas by means of stereographic drawings of this kind. In general, the viewing direction (which is stated in each case) has been chosen in such a way that the main channels are clearly visible. The unit cell has also been outlined whenever possible and provided that no changes in symmetry affecting the cell edges have been encountered. The positions of atoms (T = Si, Al) are those of the points or vertices of the net and the T-O-T bridges are represented by straight lines. The positions of the O-atoms are only approximately displayed in these diagrams since the T-O-T angles are typically around 140-150°. The idealization makes it easier to visualize the topology and basic features of zeolite framework structures which in many instances are relatively complex.

## STRUCTURE TYPE

Structural classifications of zeolites are primarily based on the topology of the frameworks. Zeolite species which do not differ with respect to the framework topology are called isotypic, i.e. they share the same structure type irrespective of composition, distribution of the different T-atoms, cell dimensions, and symmetry. A mnemonic code consisting of 3 capital letters has been adopted for each structure type following the recommendations by IUPAC on zeolite nomenclature<sup>1)</sup>.

1) "Chemical Nomenclature, and Formulation of Compositions, of Synthetic and Natural Zeolites", prepared by a special IUPAC Commission under the chairmanship of R. M. Barrer. IUPAC yellow booklet, 1978.

Structure type codes are generally derived from the names of the type species (see below) and do not include numbers and characters other than capital roman letters. Since structural criteria alone do not provide an unambiguous numbering scheme, and to facilitate later additions and simple indexing, the various structure types in this Atlas have been arranged in alphabetical order according to the structure type code. For each structure type the information given in bold type includes the full type name, the maximum topological symmetry (i.e. the maximum possible space group) and a listing of the topologically distinct T-atoms, their number per unit cell, as well as the maximum point symmetry of the respective T-sites (in square parentheses).

#### Secondary Building Units (SBU)

Zeolite frameworks can be thought to consist of finite or infinite (i.e. chain- or layer-like) component units. The finite units containing up to 16 T-atoms, which have been found to occur in framework silicates, are shown in Figure 1. These secondary building units<sup>1)</sup> are derived assuming the entire framework is made up of one type of SBU only<sup>2)</sup>. A unit cell invariably contains an integral number of SBU. Many of the frameworks can be built from several different SBU. In these cases the SBU listed in the first place is the one which occurs most frequently in related structures.

- 1) The primary building units being the single  $\text{TO}_4$  tetrahedra.
- 2) There is evidence, however, that some zeolite frameworks consist of two component units, such as 4-membered rings of silica tetrahedra which are linked to each other through single  $\text{AlO}_4$  tetrahedra as in the case of laumontite and (possibly) analcime.

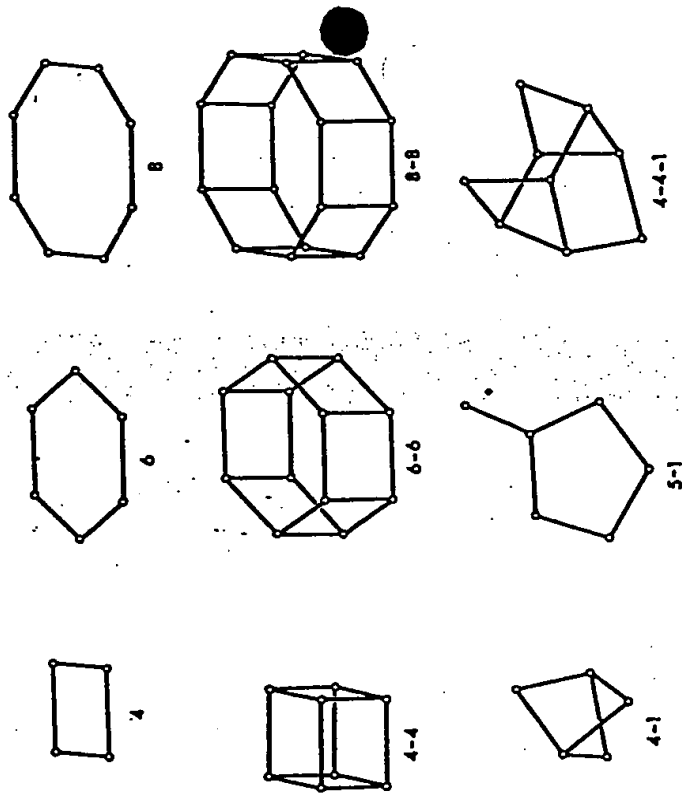


Figure 1

#### Framework Density (FD)

This is defined as the number of T-atoms per  $1000 \text{ \AA}^3$ . For zeolite frameworks structure values of at least  $20 \text{ T}/1000 \text{ \AA}^3$  are generally obtained while for zeolites the observed values range from about 1: for structures with the largest pore volume to around 20. The FD is obviously related to the pore volume but does not reflect the size of the pore openings. For some non-rigid zeolite structure types the FD values can vary appreciably. In these cases (such as glauconite) values are given for the type species and the framework in the most expanded state. The flexibility of the framework structure is to some extent displayed by the possible variation of the FD.

orthand notation has been adopted for the description of the channels in the various frameworks. Each system of equivalent channels been characterized by the channel direction (relative to the axes of the type structure) ne number of either T- or O-atoms (underlined number) forming ne smallest rings of the channels, and he crystallographic free diameters of the channels.

free diameter values are based on the atomic coordinates of the species in the hydrated state and an oxygen radius of 1.35 Å. n minimum and maximum values are given for non-circular apertures. many instances the corresponding interatomic distance vectors are approximately co-planar, and closer inspection of the diagrams ould give some information on this in the first instance. It should be noted that crystallographic free diameters depend on the state composition of the zeolite, and can differ appreciably for various ypic species, particularly in the case of non-rigid frameworks.

number of asterisks in the notation used indicates whether the chan-system is one-, two- or three-dimensional. Only those apertures e been taken into account which are more open than regular six nbered rings. In most cases these smaller openings simply form dows (rather than channels) connecting larger cavities. Interconnect-channel systems are separated by a double arrow ( $\longleftrightarrow$ ). A ver-1 bar (|) means that there is no direct access from one channel tem to the other.

e selected examples in Table 1 illustrate the various possibilities i the use of the notation. Cancrinite is characterized by a one-dimensional system of channels parallel to  $[001]$  or  $\underline{c}$  with circular ring apertures. In offretite the main channels form a similar system e are interconnected by channels made of 8-rings giving rise to a

3-dimensional channel sy. The channel system in m alite is es-sentially 2-dimensional, the 12-ring apertures of the main channels being somewhat elliptical. Paulingite is an example of a framework type containing two independent sets of 3-dimensional channel systems which are displaced against each other. ( $\langle 100 \rangle$  means there are chan-nels parallel to all crystallographically equivalent axes of the cubic structure, i.e. along  $\underline{x}$ ,  $\underline{y}$  and  $\underline{z}$ ). In gismondine the channels parallel to  $[100]$  together with those parallel to  $[010]$  give rise to a 3-dimensional channel system which can be pictured as an array of partially overlapping tubes.

Table 1: EXAMPLES ILLUSTRATING THE NOTATION FOR THE CRYSTALLOGRAPHIC CHARACTERIZATION OF THE CHANNEL

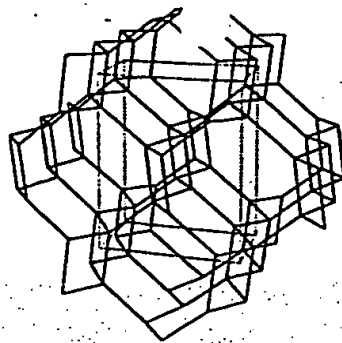
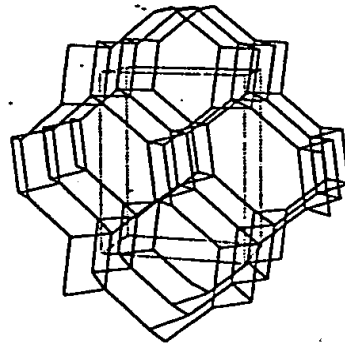
Cancrinite	$[001] \underline{12} \underline{6.2} *$
Offretite	$[001] \underline{12} \underline{6.4} * \longleftrightarrow \perp [001] \underline{8} \underline{3.6} \times \underline{5.2} **$
Mordenite	$[001] \underline{12} \underline{6.7} \times \underline{7.0} * \longleftrightarrow [010] \underline{8} \underline{2.9} \times \underline{5.7} *$
Paulingite	$\langle 100 \rangle \underline{8} \underline{3.9} *** \mid \langle 100 \rangle \underline{8} \underline{3.9} ***$
Gismondine	$\{ [100] \underline{8} \underline{3.1} \times \underline{4.4} \longleftrightarrow [010] \underline{8} \underline{2.8} \times \underline{4.9} \} ***$

#### Fault Planes (FP)

Likely FP are listed for each structure type. The existence of FP means that layer-like segments of the framework can be stacked in more than one way, giving rise to polytypism. A number of related structures (polytypes) can be readily postulated on this basis. FP also serve as an indication of possible stacking faults which may affect the critical channel dimensions.

# Type Species and References

The type species stated in the data section is the species used to establish the structure type. In the majority of cases these have been natural zeolites providing single crystal data. The composition expressed in terms of cell contents has in many cases been idealized inasmuch as compositional data give average unit cell contents which frequently correspond to fractional numbers of atoms. Isotypic species are very common and have been listed in the Index.



Li-A(BW)

Imam

8 T[m]

viewed along [001]

Secondary building units:

single 4-rings  
(single 6- or 8-rings)

Framework density:

19.0 T/1000 Å<sup>3</sup>

Channels:

[001] 8 3.6 x 4.0 \*

Fault planes:

(010), (011)

Type species:

synthetic zeolite Li-A (Barrer + White)

Li<sub>4</sub>Al<sub>4</sub>Si<sub>4</sub>O<sub>16</sub> · 4 H<sub>2</sub>O

orthorhombic, Pna2<sub>1</sub>, a=10.3 b=8.2 c=5.0 Å<sup>3</sup>)

References:

<sup>1)</sup> I. S. Kerr (1974)

## Structure Type Index

Type species are marked by an asterisk. To make the index as informative as possible all reported species and designations have been included in this section, provided the structure type assignment appears reasonably well established. Even a number of occasionally used but discredited names of mineral species have been included in this index for the afore-mentioned reason. Moreover, the inclusion of a synthetic species designation in this index must not be interpreted to mean that the designation has been formally recognized or generally accepted but merely that the material has one of the established structure types. References have been restricted to those considered necessary to identify the species. For unreferenced minerals, see Strunz (1977).

* Afghanite	AFG	G. T. Wadlinger, E. J. Rosinski, and C. J. Plank (1968)
ALPHA	LTA	
A, Na-A	LTA	D. W. Breck, W. G. Eversole, R. M. Milton, T. B. Reed and T. L. Thomas (1956)
* Analcime	ANA	
- Analcite	ANA	
B	GIS	R. M. Milton (1961)
Ba-G	LTL	R. M. Barrer and D. J. Marshall (1964)
Ba-P	KFI	R. M. Barrer, L. Hinds and E. A. D. White (1953)
Ba-Q	KFI	R. M. Barrer, L. Hinds and E. A. D. White (1953)
Barrerite	STI	E. Passaglia and D. Pongiluppi (1975)
Basic cancrinite	CAN	R. M. Barrer and E. A. D. White (1952)
Basic sodalite	SOD	R. M. Barrer and E. A. D. White (1952)
* Bikitaite	BIK	
* Brewsterite	BRE	

Ca-D	ANA	L. L. Ames and L. B. Sand (1958)
Cancrinite	CAN	
Cancrinite hydrate	CAN	J. Wyart and Michel-Lévy (1949)
Chabazite	CHA	
Clinoptilolite	HEU	A. Alberti (1975)
CsAlSiO <sub>4</sub>	ABW	S. J. Chung and Th. Hahn (1972)
D	CHA	D. W. Beck and N. A. Acara (1960)
Dachardite	DAC	
Danallite	SOD	
Desmine	STI	
Edingtonite	EDI	
Epidesmine	STI	
Epistilbite	EPI	
Erionite	ERI	
Faujasite	FAU	
Ferrierite	FER	
Garronite	GIS	G. P. L. Walker (1962)
Gismondine	GIS	
Gmelinite	GME	
Gonnardite	THO	
Harmotome	PHI	
Herschelite	CHA	
Heulandite	HEU	
Hydroxysodalite	SOD	W. Borchert and J. Heidel (1947)
(K, Ba) -G	LTL	R. M. Barrer and D. J. Marshall (1964)
Keholte	ANA	D. McConnell (1964)
K-F	EDI	R. M. Barrer and J. W. Baynham (1956)
K-M	MER	R. M. Barrer and J. W. Baynham (1956)
Laubanite	NAT	
Laumontite	LAU	
Leucite	ANA	

Leonhardite	LAU	C. T. Amirov, V. V. Dyukhin and N. V. Belov (1967)
* Levyne	LEV	
Levynite	LEV	
* Li-A	ABW	R. M. Barrer and E. A. D. White (1951)
* Linde A	LTA	D. W. Breck, W. G. Eversole, R. M. Milton, T. B. Reed and T. L. Thomas (1956)
Linde B	GIS	R. M. Milton (1961)
Linde D	CHA	D. W. Breck and N. A. Acara (1960)
* Linde L	LTL	D. W. Breck (1965); D. W. Breck and E. M. Flanigen (1968)
Linde R	CHA	R. M. Milton (1960)
Linde T	OFF-ERI	D. W. Breck and N. A. Acara (1960)
Linde W	MER	R. M. Milton (1961)
Linde X	FAU	R. M. Milton (1959)
Linde Y	FAU	D. W. Breck (1964)
* Liottite	LIO	
* Losod	LOS	W. Sieber and W. M. Meier (1974)
* Mazzite	MAZ	
* Merlinoite	MER	
* Mordenite	MOR	
N-A	LTA	R. M. Barrer and P. J. Denny (1961)
Na-B	ANA	R. M. Barrer and E. A. D. Wl. (1952)
Na-D	MOR	R. M. Barrer and E. A. D. White (1952)
Na-P1	GIS	R. M. Barrer, F. W. Bultitude and I. S. Kerr (1959)
Na-P2	GIS	R. M. Barrer, F. W. Bultitude and I. S. Kerr (1959)
* Natrolite	NAT	
Nosean	SOD	
O	OFF	R. Aiello and R. M. Barrer (1970)
* Offretite	OFF	
Omega	MAZ	E. M. Flanigen (1968)
* Paulingite	PAU	



P-[Cl]	KFI	R. M. Barrer, L. Hinds and E. A. D. White (1953)
P <sub>c</sub> , P <sub>t</sub>	GIS	A. M. Taylor and R. Roy (1964)
* Phillipsite	PHI	
P-L	LTL	E. M. Flanigen and R. W. Grose (1971)
P, Na-P	GIS	R. M. Barrer, J. W. Baynham, F. W. Bultitude, and W. M. Meter (1959)
Pollucite	ANA	
Ptilolite	MOR	
Q-[Br]	KFI	R. M. Barrer, L. Hinds and E. A. D. White (1953)
R	CHA	R. M. Milton (1960)
RbAlSiO <sub>4</sub>	ABW	S. J. Chung and Th. Hahn (1972)
* Rho	RHO	H. E. Robson, D. P. Shoemaker, R. A. Ogilvie and P. C. Manor (1973)
Scolecite	NAT	
S, Na-S	GME	R. M. Barrer, J. W. Baynham, F. W. Bultitude and W. M. Meter (1959)
* Sodallite	SOD	
Sodallite hydrate	SOD	J. Wyart and M. Michel-Lévy (1949)
Sr-D	FER	R. M. Barrer and D. J. Marshall (1964)
Sr-Q	YUG	R. M. Barrer and D. J. Marshall (1964)
Stellerite	STI	
* Stilbite	STI	
T	OFF-ERI	D. W. Breck and N. A. Acara (1960)
Tetracalcium trialuminate	SOD	V. I. Ponomarev, D. M. Khelker and N. V. Belov (1970)
* Thomsonite	THO	
* TMA-E	EAB	R. Aiello and R. M. Barrer (1970)
Tugtupite	SOD	H. Sorensen (1963)
Ultramarine	SOD	
Vlaeite	ANA	J. Mélon (1942)

W	MER	R. M. Milton (1961)
Walrakite	ANA	A. Steiner (1955)
Wellsite	PHI	P. Cerny, R. Rinaldi and R. C. S. dam (1977)
X	FAU	R. M. Milton (1959)
Y	FAU	D. W. Breck (1964)
* Yugawaralite	YUG	
Zeolon	MOR	
Zh	SOD	S. P. Zhdanov and N. N. Buntar (1971)
ZK-4	LTA	G. T. Kerr (1968)
* ZK-5	KFI	G. T. Kerr (1963)
ZK-19	PHI	G. H. Kuhl (1969)
ZK-20	LEV	G. T. Kerr (1969)
ZK-21	LTA	G. H. Kuhl (1967, 1971)
ZK-22	LTA	G. H. Kuhl (1967, 1971)
ZSM-4	MAZ	J. Ciric (1967)
* ZSM-5 <sup>1)</sup>	MFI	R. J. Argauer and G. R. Landolt (1972)
* ZSM-11	MEL	P. Chu (1973)

<sup>1)</sup> Recently, E. M. Flanigen et al (1978) reported a silica polymorph having the MFI structure type.